

Materials modelling across different scales with different tools – a perspective from the meso scale

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Abstract

Materials modelling is a field that encompasses the use of many (numerical) tools and methods and has seen great advances in recent years.

We would like to share our experience of 14,5 years of developing modelling projects and products to serve the CAE and materials modelling community – most notably models that are useful for mesoscale and macro (device) scale modelling, Discrete Element Method (DEM) and its coupling to Computational Fluid Dynamics (CFD) and most recently a python-based SaaS platform (engicloud) to connect the dots.

We would like to discuss in general how to choose the right model and tool (from 1D python models to complex 3D models) to cover different scales and requirements.

Then we would like to discuss a couple concrete application examples, such as catalytic reactors and granulation.

Finally, we will outline the need for FAIR data handling and collecting, aggregating, connecting, sharing modelling results and tools and our approach to it.